Electronic supplementary information for:

Mechanistic Insights into Excited State Intramolecular Proton Transfer in Isolated and Metal Chelated Supramolecular Biosensors.

Tolga N. V. Karsili[a,b]*, Barbara Marchetti[a,b] and Michael N. R. Ashfold[b]

[a] *Department of Chemistry, Technische Universität München, Lichtenbergstrasse 4, 85748, Garching Germany.*

[b] *School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom.*

Figure S1: Minimum energy geometries and dominant orbital excitation accompanying the lowest three singlet electronic transitions of Cd^{2+}–HDBO′ (right) and Hg^{2+}–HDBO′ (left).

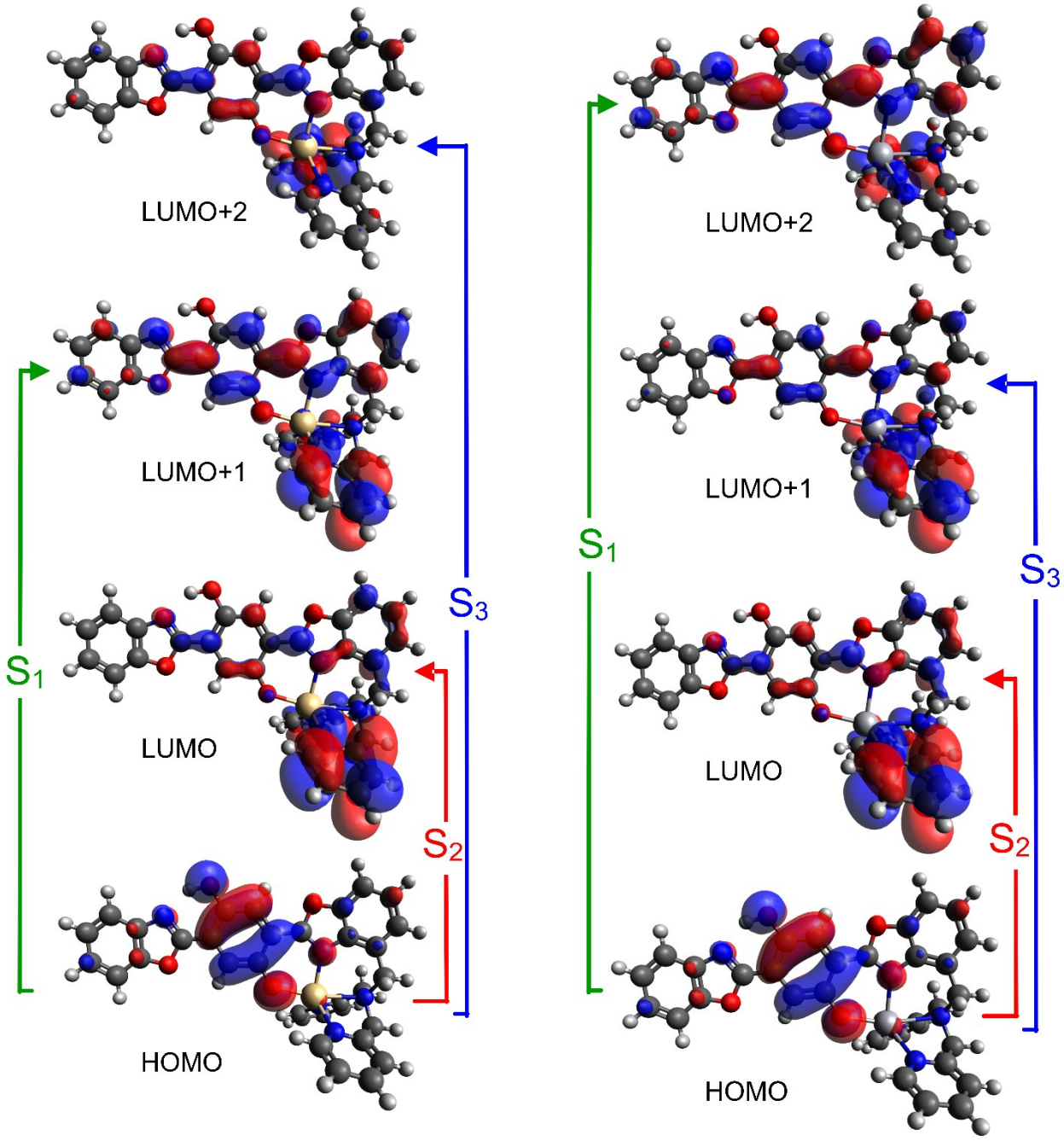

Figure S2: Magnitude and direction of the permanent dipole moment of HBO at the minimum energy geometries of (a) the S_0 state, (b) the S_1 *enol* conformer and (c) the S_1 *keto* minimum at planar geometries.